marmelolactone, II

Inchi: InChI=1S/C10H14O2/c1-7(2)4-5-9-6-8(3)10(11)12-9/h4-5,8-9H,1,6H2,2-3H3/b5-4+
InchiKey: VOJBXZDIFIJUKD-SNAWJCMRSA-N
Formula: C10H14O2
SMILES: C=C(C)C=CC1CC(C)C(=O)O1
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	12.96	kJ/mol	Joback Method
hf	-246.43	kJ/mol	Joback Method
hfus	21.76	kJ/mol	Joback Method
hvap	45.93	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.070		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
ripol	2116.00		NIST Webbook
tb	534.30	K	Joback Method
tc	756.82	K	Joback Method
tf	283.11	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.62	J/mol×K	534.30	Joback Method
cpg	350.53	J/mol×K	571.39	Joback Method
cpg	366.54	J/mol×K	608.47	Joback Method
cpg	381.64	J/mol×K	645.56	Joback Method
cpg	395.86	J/mol×K	682.64	Joback Method
cpg	409.23	J/mol×K	719.73	Joback Method
cpg	421.75	J/mol×K	756.82	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R317834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume